

Accepted Manuscript

Conditional full stability of positivity-preserving finite difference scheme for diffusion-advection-reaction models

Rafael Company, Vera N. Egorova, Lucas Jódar

PII: S0377-0427(18)30110-9
DOI: <https://doi.org/10.1016/j.cam.2018.02.031>
Reference: CAM 11537

To appear in: *Journal of Computational and Applied Mathematics*

Received date : 15 September 2017
Revised date : 22 January 2018

Please cite this article as: R. Company, V.N. Egorova, L. Jódar, Conditional full stability of positivity-preserving finite difference scheme for diffusion-advection-reaction models, *Journal of Computational and Applied Mathematics* (2018), <https://doi.org/10.1016/j.cam.2018.02.031>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Conditional full stability of positivity-preserving finite difference scheme for diffusion-advection-reaction models

Rafael Company¹, Vera N. Egorova², Lucas Jódar¹

¹ *Universitat Politècnica de València, camino de Vera s/n, 46022, Valencia, Spain*

² *BCAM - Basque Center for Applied Mathematics, Al. de Mazarredo 14, 48009 Bilbao, Basque Country, Spain*

Abstract

The matter of the stability for multidimensional diffusion-advection-reaction problems treated with the semi-discretization method is remaining challenge because when all the stepsizes tend simultaneously to zero the involved size of the problem grows without bounds. Solution of such problems is constructed by starting with a semi-discretization approach followed by a full discretization using exponential time differencing and matrix quadrature rules. Analysis of the time variation of the numerical solution with respect to previous time level together with the use of logarithmic norm of matrices are the basis of the stability result. Sufficient stability conditions on stepsizes, that also guarantee positivity and boundedness of the solution, are found. Numerical examples in different fields prove its competitiveness with other relevant methods.

Keywords: Diffusion-advection-reaction, semi-discretization, exponential time differencing, finite difference, numerical analysis.

2010 MSC: 65M06, 65M12, 65M20

1. Introduction

Time-dependent diffusion-advection-reaction (DAR) models have application in a wide class of problems [1] appearing in many fields as fluid dynamics [1], biology [2], population dynamics [3], and financial mathematics [4], etc. Such time evolution problems are modeled by involving three factors: diffusion, advection and reaction. Diffusion deals with the dispersion given in the species involved in the process throughout the domain of the problem. Advection is

related to the movement of species due to the fluid transport medium and the reaction explains the interaction through which the species are generated or
10 consumed [5].

The partial differential equation (PDE) that governs the diffusion-advection-reaction type processes adds significant mathematical complexity to be considered carefully when solving the problem. Well-posedness conditions for nonlinear second order PDEs problems including DAR initial value problems are given
15 in Section 4.9 of [6]. The notion of viscosity solutions provides a framework in which existence and uniqueness theorems may be proved by very efficient arguments. A rigorous study can be found in [7] for initial boundary second order PDEs.

It is important to point out that existence and uniqueness conditions uses
20 to be much more restrictive than they appear frequently in practice. Even when such conditions are not fulfilled, the search of numerical solutions is important because the practitioners may have empirical evidences of the problem to check the reliability of the approximation.

Only in some particular cases it is possible to solve the DAR equations
25 exactly [8]. In a more general situation, numerical techniques are required. One of the common methods is a semi-discretization with respect to spatial variables achieving a system of ordinary differential equations (ODE). It is a fertile approach allowing two further alternatives. For the numerical solution of the systems of ODEs there are many numerical methods available, such as
30 Runge-Kutta methods [9] or the further time discretization deriving many types of finite difference schemes [1, 10, 11].

Alternative approach, that it is used in the present study, is the exact integration of the semi-discretized equations using the Exponential Time Differencing (ETD) method [12] involving an integral term that needs to be approximated
35 because is expressed in terms of the unknown solution of the semi-discretized system of ODEs, that it has been recently treated in [13]. This approach has to afford the challenge of the computation of the inverse of matrices not always well conditioned when eigenvalues are close to zero [14].

Dealing with numerical finite difference methods, as the best model may
 40 be wasted with careless analysis, it is convenient to study the stability of the
 numerical solution as all the stepsize tends to zero. However, as the spatial
 stepsize tends to zero the dimension of the matrix of the semi-discretized system
 of ODEs grows without end becoming a mathematical challenge. Apart from the
 stability, as the solutions of the problems represent concentrations, populations
 45 or prices, the positivity is a necessary requirement for many practical problems.

In this paper we consider multidimensional heterogeneous DAR problems of
 the type

$$\frac{\partial u}{\partial t} = \sum_{i=1}^M D_{ii}(\mathbf{x}) \frac{\partial^2 u}{\partial x_i^2} + \sum_{i=1}^M \alpha_i(\mathbf{x}) \frac{\partial u}{\partial x_i} + F(\mathbf{x}, u), \quad (1)$$

where $(\mathbf{x}, t) \in \Omega \times (0, T) \subset \mathbb{R}^{M+1}$, together with the non-negative initial and
 boundary conditions

$$u(\mathbf{x}, 0) = U_0(\mathbf{x}) \leq 1, \mathbf{x} \in \Omega, \quad u(\mathbf{x}, t) = \phi(\mathbf{x}, t) \leq 1, \mathbf{x} \in \partial\Omega, \quad (2)$$

50 where diffusion and advection coefficients $D_{ii}(\mathbf{x})$ and $\alpha_i(\mathbf{x})$ are continuous func-
 tions for $1 \leq i \leq M$ and $D_{ii}(\mathbf{x}) > 0$. The source term $F(\mathbf{x}, u)$ is positive admit-
 ting bounded partial derivatives $|\frac{\partial F}{\partial u}(\mathbf{x}, u)| \leq \lambda$, $0 \leq u \leq 1$, and $F(\mathbf{x}, 1) = 0$,
 $x \in \Omega$.

In this paper a semi-discretization method to solve (1)-(2) is presented to-
 55 gether with a ETD scheme for the integration of the resulting system of ODEs
 using the accurate Simpson's rule and avoiding the calculation of the inverse
 of the coefficient matrix of the system. Furthermore, taking advantage of log-
 arithmic norm of matrices and found properties of matrix exponential of the
 coefficient matrix a stability analysis is performed to guarantee conditionally
 60 the boundedness of the solution independently of the size of the semi-discrete
 system.

This paper is organized as follows. Section 2 addresses the spatial semi-
 discretization and further proposed ETD scheme construction. Positivity and
 stability analysis is included into Section 3. In Section 4, a couple of numer-

65 ical examples dealing with Fisher-Kolmogorov-Petrovsky-Piscounov equation in Population Dynamics and Multi-asset American basket option in Financial Mathematics are included in order to illustrate the use of the proposed scheme.

2. Semi-discretization and ETD scheme

The numerical solution is constructed in the computational domain with limits $x_{i_{\min}}$ and $x_{i_{\max}}$, $i = 1, \dots, M$. A uniform mesh in each coordinate spatial computational grid of $N_i + 1$ nodes with stepsizes h_i takes the following form

$$\xi_i^j = x_{i_{\min}} + jh_i, \quad h_i = \frac{x_{i_{\max}} - x_{i_{\min}}}{N_i}, \quad 0 \leq j \leq N_i, \quad 1 \leq i \leq M. \quad (3)$$

An approximate solution at the point $(\boldsymbol{\xi}^j, t) = (\xi_1^{j_1}, \xi_2^{j_2}, \dots, \xi_M^{j_M}, t)$ is denoted by $u_{j_1, \dots, j_M} = u_{j_1, \dots, j_M}(t)$. Let us denote the set of all mesh points by Γ , the subset of the mesh points located at the boundary of the numerical domain by

$$\partial\Gamma = \left\{ (\xi_1^{j_1}, \xi_2^{j_2}, \dots, \xi_M^{j_M}) \mid \exists m, 1 \leq m \leq M, j_m = 0 \text{ or } j_m = N_m \right\}, \quad (4)$$

and the subset of interior nodes by $\mathring{\Gamma} = \Gamma \setminus \partial\Gamma$. Then semi-discretization of the equation (1) is obtained by using the second order central difference approximation for the spatial derivatives, resulting in the system of ODEs of the form

$$\begin{aligned} \frac{du_{j_1, \dots, j_M}}{dt} = & \sum_{i=1}^M D_{ii}(\boldsymbol{\xi}^j) \frac{u_{j_1, \dots, j_i-1, \dots, j_M} - 2u_{j_1, \dots, j_i, \dots, j_M} + u_{j_1, \dots, j_i+1, \dots, j_M}}{h_i^2} \\ & + \sum_{i=1}^M \alpha_i(\boldsymbol{\xi}^j) \frac{u_{j_1, \dots, j_i+1, \dots, j_M} - u_{j_1, \dots, j_i-1, \dots, j_M}}{2h_i} + F(\boldsymbol{\xi}^j, u_{j_1, \dots, j_M}). \end{aligned} \quad (5)$$

70 Let us introduce the following notation for $i = 1, \dots, M$:

$$h_i = \beta_i h, \quad D_{ii}(\boldsymbol{\xi}^j) = \sum_{i=1}^M \frac{D_{ii}(\boldsymbol{\xi}^j)}{\beta_i^2}, \quad (6)$$

$$a_0^j = -\frac{2}{h^2} D(\boldsymbol{\xi}^j), \quad (7)$$

$$a_{\pm i}^j = \frac{1}{h^2} \left(\frac{D_{ii}(\boldsymbol{\xi}^j)}{\beta_i^2} \pm \frac{h}{2\beta_i} \alpha_i(\boldsymbol{\xi}^j) \right). \quad (8)$$

Let us denote by $\mathbf{u} = \mathbf{u}(t) \in \mathbb{R}^{N+1}$ the vector of all values u_{j_1, \dots, j_M} , such that $\mathbf{u} = [u_0, \dots, u_N]^T$, where $N + 1$ means the total number of mesh points and each index j , $0 \leq j \leq N$, has a one to one correspondence with the set of indexes $[j_1, \dots, j_M]$ as follows

$$N + 1 = \prod_{i=1}^M (N_i + 1) = \frac{1}{h^M} \prod_{i=1}^M \frac{x_{i_{\max}} - x_{i_{\min}} + \beta_i h}{\beta_i}, \quad (9)$$

$$[j_1, \dots, j_M] \equiv j = j_1 + \sum_{m=2}^M \left(\prod_{n=1}^{m-1} (N_n + 1) \right) j_m. \quad (10)$$

System (5) with the boundary and initial conditions (2) can be presented in the following vector form

$$\frac{d\mathbf{u}}{dt}(t) = \mathbf{A}\mathbf{u}(t) + \mathbf{f}(\boldsymbol{\xi}, \mathbf{u}); \quad \mathbf{u}(0) = [u_0(0), \dots, u_N(0)]^T, \quad (11)$$

where $\mathbf{f}(\boldsymbol{\xi}, \mathbf{u}) = [f_0, \dots, f_N]^T$, $f_j = F(\boldsymbol{\xi}^j, \mathbf{u})$, if $\boldsymbol{\xi}^j \in \mathring{\Gamma}$ and $f_j = \frac{\partial \phi(\boldsymbol{\xi}^j, t)}{\partial t}$ otherwise, $u_j(0) = U_0(\boldsymbol{\xi}^j)$, $j = 0, \dots, N$.

Matrix A is a sparse banded $(N + 1) \times (N + 1)$ matrix whose size depends on stepsize h (see eq. (9)), and rows are entirely with zeros or containing $2M + 1$ non-zero entries. In fact, $A = (a_{ij})_{0 \leq i, j \leq N}$, with only non-zero entries for $\boldsymbol{\xi}^i \in \mathring{\Gamma}$, such that

$$a_{ii} = a_{\pm 0}^i, \quad a_{i, i \pm 1} = a_{\pm 1}^i, \quad a_{i, i \pm \prod_{n=1}^{m-1} (N_n + 1)} = a_{\pm m}^i, \quad 2 \leq m \leq M. \quad (12)$$

Numerical solution of the system (11) is constructed by the ETD method [12]. Let us introduce temporal discretization with the fixed constant time step $k = \frac{T}{N_t}$, so $t^n = nk$, $n = 0, \dots, N_t - 1$. Then the exact solution of the system of ODE (11) in some given interval $t \in [t^n, t^{n+1}]$ is given by Section 2.1 of [12]:

$$\mathbf{u}(t^{n+1}) = e^{Ak} \mathbf{u}(t^n) + \int_0^k e^{As} \mathbf{f}(\boldsymbol{\xi}, \mathbf{u}(t^{n+1} - s)) ds. \quad (13)$$

We propose a first explicit approximation of the integral in (13) by replacing $\mathbf{u}(t^{n+1} - s)$ by the known value $\mathbf{u}(t^n)$ corresponding to $s = k$. Let us denote \mathbf{v}^{n+1} by

$$\mathbf{v}^{n+1} = e^{Ak} \mathbf{u}(t^n) + \left(\int_0^k e^{As} ds \right) \mathbf{f}(\boldsymbol{\xi}, \mathbf{u}(t^n)), \quad (14)$$

then in accordance with Section 2.1 of [12], the local truncation error is $O(k^2)$.

Instead of solving the integral $\int_0^k e^{As} ds$ in exact form involving A^{-1} like [15], as matrix A can be singular or ill-conditioned, we use the accurate Simpson's rule, see [16],

$$\int_0^k e^{As} ds = k\varphi(A, k) + O(k^5), \quad \varphi(A, k) = \frac{1}{6} \left(I + 4e^{A\frac{k}{2}} + e^{Ak} \right). \quad (15)$$

Let $\mathbf{u}^n \approx \mathbf{u}(t^n)$ be the numerical solution of the proposed fully discretized explicit scheme

$$\mathbf{u}^{n+1} = e^{Ak}\mathbf{u}^n + k\varphi(A, k)\mathbf{f}(\boldsymbol{\xi}, \mathbf{u}^n), \quad t^n = nk, \quad n = 0, \dots, N_t - 1. \quad (16)$$

According to (15) the local truncation error of the full discretized explicit
75 scheme (16) versus the ODE system (11) is of the second order in time.

3. Positivity and stability

In this section we pay attention to the stability in the infinity norm of the scheme (16) in the classical sense, i.e. that the numerical solution \mathbf{u}^n remains bounded at each time level n , such that, $\|\mathbf{u}^n\|_\infty \leq C$, $0 \leq n \leq N_t$, where C
80 is independent of the stepsizes h and k . For the proposed scheme the stability analysis is a challenging task, because the dimension of the matrix A grows as stepsizes decrease (see (3)) and the entries of the matrix A also grows (see (8)).

For the sake of clarity in the presentation we recall some definitions and results that might be found in [17].

A matrix $A \in \mathbb{R}^{n \times n}$ is called the Metzler matrix if its off-diagonal entries are non-negative. If A is the Metzler matrix, then $e^{At} \geq 0$ for $t \geq 0$. It is well known the boundedness of exponential matrix norm by the exponential of the logarithmic norm $\mu[A]$, [18]:

$$\|e^{Ak}\| \leq e^{k\mu[A]}. \quad (17)$$

Denoting the real part of complex number x by $\Re(x)$, $\mu_\infty[A]$ can be calcu-

lated as follows, see [19], p. 33,

$$\mu_\infty[A] = \max_i \left(\Re(a_{ii}) + \sum_{j \neq i} |a_{ij}| \right). \quad (18)$$

From (8) coefficients $a_{\pm i}^j$, $i = 1, \dots, M$, are non-negative, and correspondingly matrix A is Metzler, if stepsize h is chosen as

$$h \leq \min_{1 \leq i \leq M} \frac{2D_{ii}(\mathbf{x})}{\beta_i |\alpha_i(\mathbf{x})|}, \quad \mathbf{x} \in \Omega. \quad (19)$$

From (8), (12) and (18), one gets $\mu_\infty[A] = 0$.

Thus, from (17) $\|e^{Ak}\|_\infty \leq e^0 = 1$. And from (15), $\|\varphi(A, k)\|_\infty \leq 1$. A has several zero rows, and their corresponding rows in e^{Ak} have only one entry equal to 1 while the other entries are zeros, then

$$\|e^{Ak}\|_\infty = \|\varphi(A, k)\|_\infty = 1, \quad (20)$$

The non-negativity of \mathbf{u}^n follows from the property of the Metzler matrix A , that is the exponential e^{Ak} is non-negative, and non-negativity of the source term and $\varphi(A, k)$. The boundedness of the solution ($u_i^n \leq 1$, $0 \leq i \leq N$, $0 \leq n \leq N_t$) is proven by using the induction principle. Let us represent (16) as a function g_i on the arguments u_0^n, \dots, u_N^n , given by

$$u_i^{n+1} = g_i(u_0^n, \dots, u_N^n) = (e^{Ak})_i \mathbf{u}^n + k (\varphi(A, k))_i \mathbf{f}(\boldsymbol{\xi}, \mathbf{u}^n). \quad (21)$$

Assuming the boundedness of the derivative $|\frac{\partial F}{\partial u}| \leq \lambda$, $x \in \Omega$, $0 \leq u \leq 1$, then from non-negativity of e^{Ak} and $\varphi(A, k)$ one gets

$$\frac{\partial g_i}{\partial u_j^n} \geq (e^{Ak})_{ij} - k\lambda (\varphi(A, k))_{ij}, \quad 0 \leq i, j \leq N. \quad (22)$$

Let us denote $\Psi(A, k) = e^{Ak} - k\lambda\varphi(A, k)$, and the vector function

$$g(u_i^n, \dots, u_N^n) = [g_1, \dots, g_N]^T, \quad (23)$$

then from (22) the Jacobian matrix $\frac{\partial g}{\partial \mathbf{u}^n}$ satisfies

$$\frac{\partial g}{\partial \mathbf{u}^n} \geq \Psi(A, k). \quad (24)$$

Let us denote

$$a_0 = \min_{0 \leq j \leq N} a_0^j. \quad (25)$$

Note that the non-negativity of $\Psi(A, k)$ guarantees the non-negativity of $\frac{\partial g}{\partial u^n}$ and hence, g_i increases in each direction u_j^n . In fact, from (8) and under condition (19), $B = A - a_0 I$ verifies $B \geq 0$, and taking into account that $e^{Ak} = e^{a_0 k} e^{Bk}$, $\Psi(A, k)$ can be written as follows

$$\Psi(A, k) = \phi_0(k)I + \sum_{s=1}^{\infty} \phi_s(k) \frac{B^s k^s}{s!}, \quad (26)$$

$$\phi_0(k) = e^{a_0 k} - \frac{k\lambda}{6} \left(1 + 4e^{a_0 \frac{k}{2}} + e^{a_0 k} \right), \quad (27)$$

$$\phi_s(k) = e^{a_0 k} - \frac{k\lambda}{6} \left(\frac{4}{2^s} e^{a_0 \frac{k}{2}} + e^{a_0 k} \right). \quad (28)$$

Taylor expansion of (27) shows that for some ξ , such that $0 < \xi < k$,

$$\begin{aligned} \phi_0(k) &= 1 - k(\lambda - a_0) + k^2 \frac{\phi_0''(\xi)}{2}, \\ \phi_0''(\xi) &= a_0^2 e^{a_0 \xi} + \frac{\lambda}{3} |a_0| e^{a_0 \frac{\xi}{2}} + \frac{\lambda |a_0|}{6} (2 - |a_0| \xi) \left(e^{a_0 \xi} + e^{a_0 \frac{\xi}{2}} \right). \end{aligned} \quad (29)$$

Note that the sum of the two first terms of the Taylor expansion of $\phi_0(k)$, $1 - k(\lambda - a_0)$ is positive, if $k < \frac{1}{\lambda + |a_0|}$, and by (8) this occurs when

$$k < \frac{h^2}{2d + \lambda h^2}, \quad d = \max_{\mathbf{x} \in \Omega} D(\mathbf{x}). \quad (30)$$

Condition (30) implies $2 - |a_0| \xi > 0$ and from (29), $\phi_0''(\xi)$ and $\phi_0(k)$ are positive. It is easy to check that for $s \geq 1$, $\phi_s(k) \geq \phi_0(k) > 0$. Thus, Jacobian matrix $\frac{\partial g}{\partial u^n}$ is non-negative, and using induction hypothesis $u_i^n \leq 1$ and (21), non-negativity of u_i^n and $F(x, 1) = 0$, $x \in \Omega$, under conditions (19) and (30) for the interior points one gets

$$0 \leq u_i^{n+1} = g_i(u_0^n, \dots, u_N^n) \leq g_i(1, \dots, 1) = \|(e^{Ak})_i\|_{\infty} \leq \|e^{Ak}\|_{\infty} = 1. \quad (31)$$

Summarizing all above, the main result of the paper is established as follows

Theorem 3.1. *With previous notation under conditions (19) and (30) the numerical solution \mathbf{u}^n of the scheme (16) is non-negative and $\|\cdot\|_{\infty}$ -stable, with*

$$\|\mathbf{u}^n\|_{\infty} \leq 1 \text{ at any time level } 0 \leq n \leq N_t. \quad 90$$

4. Applications and simulations

In this section we present two multidimensional DAR problems to illustrate the proposed ETD technique.

4.1. Fisher-Kolmogorov-Petrovsky-Piscounov equation

A generalized diffusive logistic model finds an application in many fields. For two spatial dimensions it takes the form of the well known 2D Fisher-Kolmogorov-Petrovsky-Piscounov equation [20, 21]

$$\frac{\partial u}{\partial t} = a \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + f(u), \quad (32)$$

where the unknown $u(x, y, t)$ represents the distribution density of a species expressed as a function of the spatial coordinates x, y , and time t . Here $a > 0$ is the diffusion coefficient, $f(u) = bu(1 - u^p)$ is the source term with $b > 0$ and $p \geq 1$. Without loss of generality, we take $a = b = 1$. Following the method in [22], initial and boundary conditions are defined by a family of the travelling wave solutions with the arbitrary real numbers φ and C given in [23].

$$u^\pm(x, y, t) = \left[\frac{1}{2} \tanh \psi + \frac{1}{2} \right]^{2/p}, \quad (33)$$

$$\psi = \pm \frac{p}{2\sqrt{2p+4}}(x \sin \varphi + y \cos \varphi) + \frac{p(p+4)}{4(p+2)}t + C. \quad (34)$$

Example 1. Let us consider Fisher-KPP equation with the parameters given in Table 1 for the cases a) and b) correspondingly, as it is proposed in [23]. In both cases the computational domain is a square symmetric with respect to x and y axes, such that $x_{\min} = y_{\min} = -x_{\max} = -y_{\max}$. The spatial discretization is presented by the uniform grid $h_1 = h_2 = h$.

The numerical solution for both examples is presented in Figures 1 and 2. The solid surface corresponds to the initial condition, the wireframe mesh correspond to the solution at the moment $t = T$.

	p	x_{\max}	T	\pm	C	φ	h	k
Example 1.a)	1	20	10	-	$-\ln \sqrt{10}$	$\frac{3}{4}\pi$	1.00	0.01
Example 1.b)	2	30	15	+	$-\ln \sqrt{5}$	$\frac{2}{3}\pi$	2.00	0.02

Table 1: Parameters in Example 1.

h	k		
	10^{-1}	10^{-2}	10^{-4}
4	2.8985e-03	1.2824e-03	1.1425e-03
2	2.4343e-03	4.8579e-04	3.2553e-04
1	2.3595e-03	2.8714e-04	8.5989e-05
0.5	2.3206e-03	2.5000e-04	2.2995e-05

Table 2: Relative errors of the numerical solution with respect to the exact solution at $t = 1$ in Example 1.a).

The relative error at $t = 1$ for the numerical solution by the proposed ETD method in Example 1.a) is presented in Table 2. Results demonstrate competitive accuracy with respect to the semi-explicit finite difference methods proposed in [23].

4.2. Multi-asset American basket option

The considered approach can be applied to multi-dimensional Black-Scholes (BS) equation. Let S_1, \dots, S_M be the asset prices, where M is the number of assets in a portfolio. Let us denote the vector of asset prices $\mathbf{S} = (S_1, \dots, S_M)^T$ and $P(\mathbf{S}, \tau)$ be the value of American basket option at the moment τ , where τ is time to maturity T , with the payoff function

$$P(\mathbf{S}, 0) = \left(E - \sum_{i=1}^M \alpha_i S_i \right)^+, \quad (35)$$

where E is the strike price and α_i is the positive weight of the corresponding i -th asset in the basket. Assuming that the asset prices follow a geometric Brownian

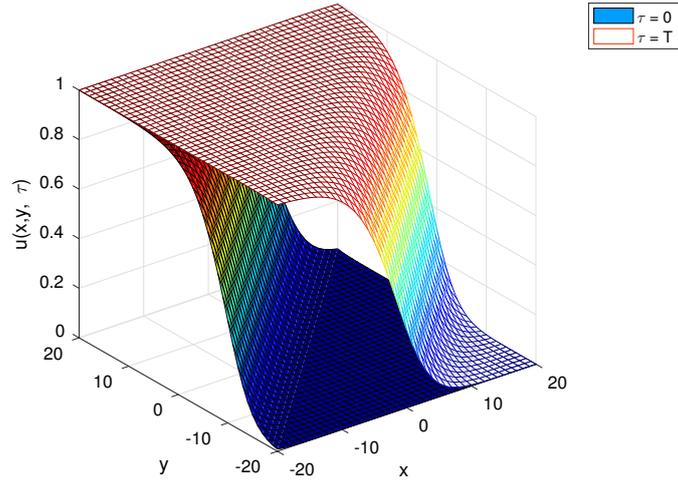


Figure 1: Example 1.a).

motion, using Martingale strategies, no-arbitrage principle and Itô's calculus
 125 (see [24]), the option price $P(\mathbf{S}, \tau)$ is the solution of the following PDE problem

$$\frac{\partial P}{\partial \tau} = \frac{1}{2} \sum_{i=1, j=1}^M \rho_{ij} \sigma_i \sigma_j S_i S_j \frac{\partial^2 P}{\partial S_i \partial S_j} + \sum_{i=1}^M (r - q_i) S_i \frac{\partial P}{\partial S_i} - rP + F(P), \quad (36)$$

$$S_i > 0, \quad i = 1, \dots, M, \quad 0 < \tau \leq T,$$

where σ_i is the volatility of S_i , ρ_{ij} is the correlation between S_i and S_j , r is the risk-free rate, q_i is the constant dividend yield of i -th asset.

Let us denote matrix $R \in \mathbb{R}^{M \times M}$ as the correlation matrix with entries ρ_{ij} , satisfying $-1 \leq \rho_{ij} \leq 1$. The nonlinear penalty term $F(P)$ has several suitable forms [25, 26]. Here we chose the following type, see [25],

$$F(P) = \lambda (P(\mathbf{S}, 0) - P(\mathbf{S}, \tau))^+, \quad (37)$$

where λ is non-negative. This penalty term is in accordance with recent rationality parameter approach [27, 28], that takes into account that the buyer does
 130 not exercise when it is not profitable.

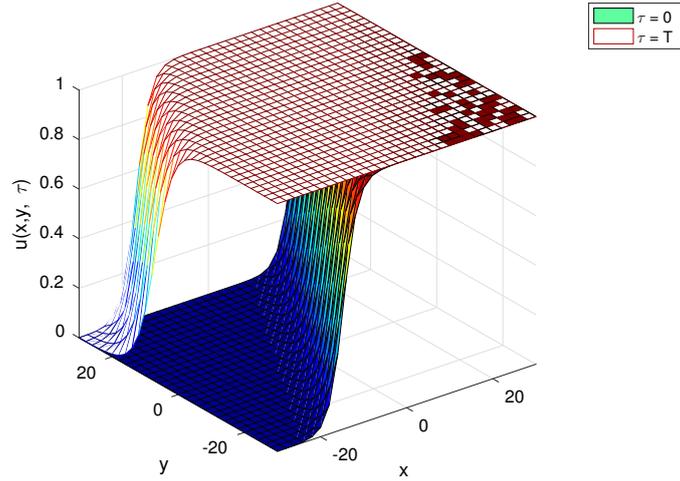


Figure 2: Example 1.b) .

Note that at each boundary $S_i = 0$ the Black-Scholes equation for $M - 1$ assets is established and

$$\lim_{S_i \rightarrow \infty} P(S_1, \dots, S_i, \dots, \tau) = 0, \quad 1 \leq i \leq M. \quad (38)$$

In the case of two underlying assets after the cross-derivative elimination proposed in [29] and following notation therein, (36) takes the DAR problem form

$$\begin{aligned} \frac{\partial U}{\partial \tau} &= \frac{1}{2} \frac{\partial^2 U}{\partial y_1^2} + \frac{1}{2} (1 - \rho^2) \frac{\partial^2 U}{\partial y_2^2} + \delta_1 \frac{\partial U}{\partial y_1} \\ &+ (\delta_2 - \rho \delta_1) \frac{\partial U}{\partial y_2} - rU + \lambda (U(\mathbf{y}, 0) - U(\mathbf{y}, \tau))^+, \end{aligned} \quad (39)$$

where $(y_1, y_2) \in \mathbb{R}^2$, $0 < \tau \leq T$, and

$$y_1 = \frac{1}{\sigma_1} \ln \frac{S_1}{E}, \quad y_2 = \frac{1}{\sigma_2} \ln \frac{S_2}{E} - \frac{\rho}{\sigma_1} \ln \frac{S_1}{E}, \quad U(y_1, y_2, \tau) = \frac{1}{E} P(S_1, S_2, \tau). \quad (40)$$

135 Initial condition takes the following form

$$U(y_1, y_2, 0) = \left(1 - \alpha_1 e^{\sigma_1 y_1} - \alpha_2 e^{\sigma_2 (y_2 + \rho y_1)}\right)^+. \quad (41)$$

Numerical solution is found in bounded domain $[y_{1\min}, y_{1\max}] \times [y_{2\min}, y_{2\max}]$, such that boundary conditions are fulfilled.

Then the semi-discretized in space approximation of (39) takes the following five-point stencil form

$$\begin{aligned} \frac{du_{i,j}}{d\tau} = & a_{-2}u_{i,j-1} + a_{-1}u_{i-1,j} + a_0u_{i,j} + a_1u_{i+1,j} + a_2u_{i,j+1} \\ & + \lambda(u_{i,j}(0) - u_{i,j}(\tau))^+, \end{aligned} \quad (42)$$

140 where the coefficients a_0 and $a_{\pm i}$ are

$$a_0 = -\frac{1}{h^2} \left(\frac{1}{\beta_1^2} + \frac{1 - \rho^2}{\beta_2^2} + rh^2 \right), \quad a_{\pm 1} = \frac{1}{h^2} \left(\frac{1}{2\beta_1^2} \pm \frac{h\delta_1}{2\beta_1} \right), \quad (43)$$

$$a_{\pm 2} = \frac{1}{h^2} \left(\frac{1 - \rho^2}{2\beta_2^2} \pm \frac{h}{2\beta_2} (\delta_2 - \rho\delta_1) \right). \quad (44)$$

In this case we include the linear reaction term $-ru$ into the homogeneous part $\mathbf{A}\mathbf{u}$ of equation (11), because the matrix A remains a Metzler one and the nonlinear source term is non-negative. Theorem 3.1 is applied to (42), the nonlinear source term (37) admitting piecewise bounded derivative with respect
145 to P , or U after the transformation. In this case stability condition (30) takes the form

$$k < \frac{h^2}{d + (r + \lambda)h^2}, \quad d = \frac{1}{\beta_1^2} + \frac{1 - \rho^2}{\beta_2^2}. \quad (45)$$

Next, we present some numerical results. Example 2 shows that the stability condition (45) is crucial: if the condition is broken, the numerical results can be wrong. The implementation of the proposed method has been done by using
150 MatLAB R2015a on processor Pentium(R) Dual-Core CPU E5700 3.00 GHz. The results of the following examples are presented in original variables (\mathbf{S}, τ) obtained by the inverse transformation.

Example 2. We consider American basket put option with no dividends payments pricing with the following parameters

$$\sigma_1 = 0.65, \sigma_2 = 0.25, r = 0.05, \rho = 0.1, \alpha_1 = \alpha_2 = 0.5, T = 1, E = 9. \quad (46)$$

The penalty parameter is chosen $\lambda = 100$, $\beta_1 = \beta_2 = 1$. Transformed computational domain is $[-8, 8] \times [-8, 8]$. In Figures 3 and 4 the option price is presented for various h and according to (45), fixed $k = 8 \cdot 10^{-3}$. If time step is chosen larger, for example, $k = 0.05$ or $k = 0.1$ (see Figures 5 and 6), the solution exceeds the strike value E , which does not agree with reality.

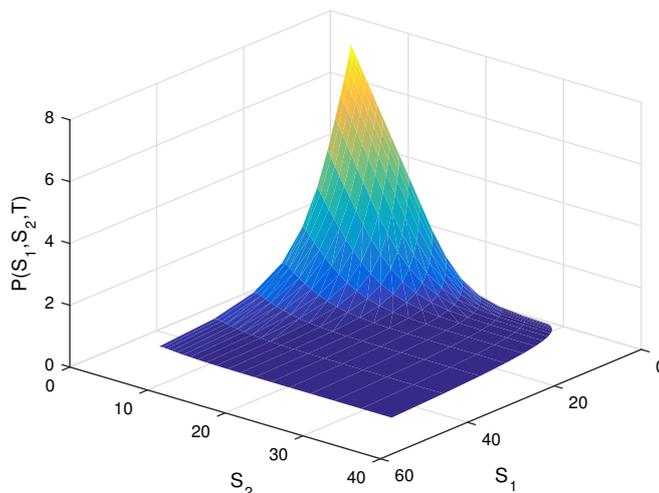


Figure 3: Reliable basket option price of Example 2 at $\tau = T$ for $h = 0.5$.

Example 3 deals with comparison between the proposed scheme and the tree method of [30]. Influence of the parameter λ to the solution is also studied.

Example 3. The American basket put option of two assets is considered with the following parameters [30]

$$\sigma_1 = 0.3, \sigma_2 = 0.2, r = 0.05, \rho = 0.6, \alpha_1 = 0.7, \alpha_2 = 0.3, T = 1, E = 50. \quad (47)$$

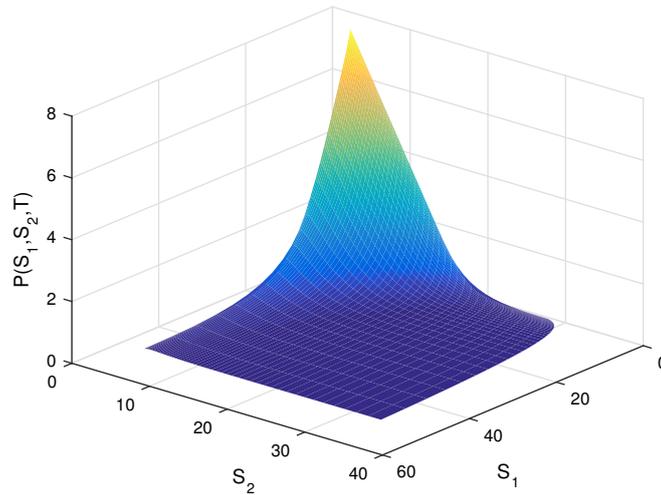


Figure 4: Reliable basket option price of Example 2 at $\tau = T$ for $h = 0.2$.

160 As a reference value at the point $\mathbf{S} = (50, 50)$ the result of the Binomial Tree method of [30] is used. The results of the proposed method with various spatial stepsizes h and fixed $k = 5 \cdot 10^{-3}$, in the computational spatial domain $[-8, 8] \times [-8, 8]$ are presented in Table 3.

h	Number of nodes	Value	Ratio
0.8	21×21	3.7075	
0.4	41×41	3.9537	12.5047
0.2	81×81	3.9730	10.1905
0.1	161×161	3.9747	5.2500
Tree method (P)		3.9751	

Table 3: Comparison of option price for Example 3.

The convergence ratio is the factor by which the error decreases at each grid refinement. It is presented in Table 3, where the absolute error is computed as

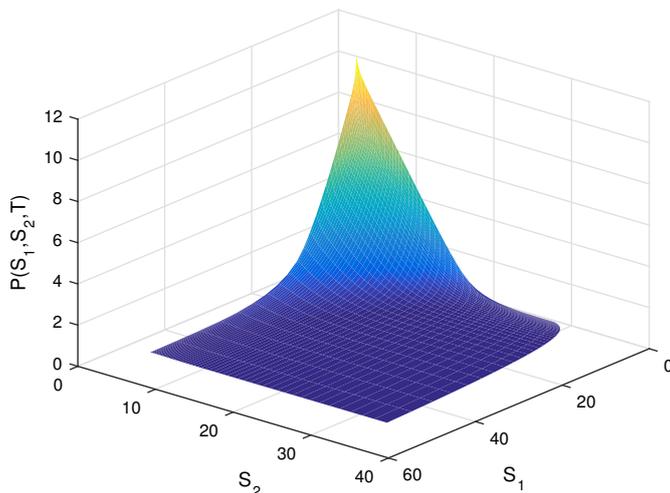


Figure 5: Wrong basket option price of Example 2 at $\tau = T$ with broken stability conditions ($k = 0.05$, $h = 0.2$).

follows

$$\epsilon_h = |P_h - P|, \quad (48)$$

where P_h is the computed value of the option, P is the reference value obtained
 165 by the tree method in [30]. The error ϵ is plotted for various stepsizes h in
 Figure 7.

The choice of timestep k depends on the value of the parameter λ . In Table
 4 values of the basket option with parameters (47) at $\mathbf{S} = (50, 50)$ applying
 fixed spatial stepsize $h = 0.2$ are presented depending on λ .

170 The numerical simulations of Example 3 show that the accuracy remains
 almost fixed for values of $\lambda > 100$. It is advisable to chose λ about 100 to save
 the computational time.

The proposed method can be applied not only for put options, but also for

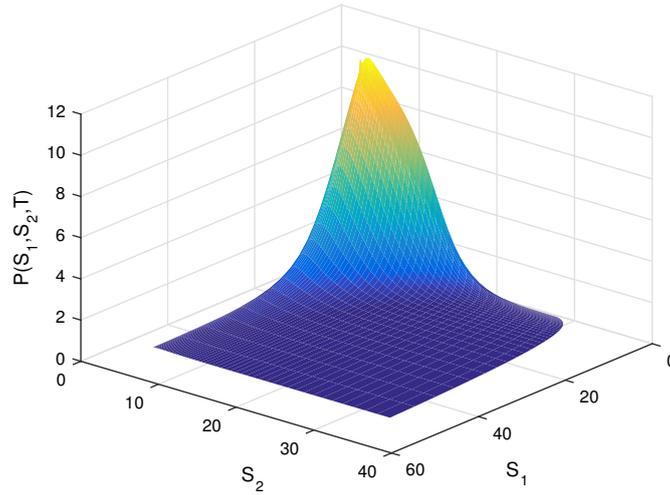


Figure 6: Wrong basket option price of Example 2 at $\tau = T$ with broken stability conditions ($k = 0.1$, $h = 0.2$).

call options. Initial condition in this case takes the following form

$$P(\mathbf{S}, 0) = \left(\sum_{i=1}^M \alpha_i S_i - E \right)^+. \quad (49)$$

Example 4 provides numerical solution for American basket call option and its comparison with high order finite element method of [15].

Example 4. *The American basket call option of two assets with the strike price $E = 100\$$ is considered with the following parameters [15]*

$$\sigma_1 = 0.12, \sigma_2 = 0.14, r = 0.03, \rho = 0.3, q_1 = 0.01, q_2 = 0.01, T = 0.5. \quad (50)$$

175 In Table 5 we include the results at $\mathbf{S} = (100, 100)$ for $\lambda = 100$, various spatial stepsizes h and corresponding k under condition (30). The numerical solution by high-order computational method of [15] is denoted by HOC. The numerical solution at $\tau = T$ and the payoff for American basket call options are presented in Figures 8 and 9.

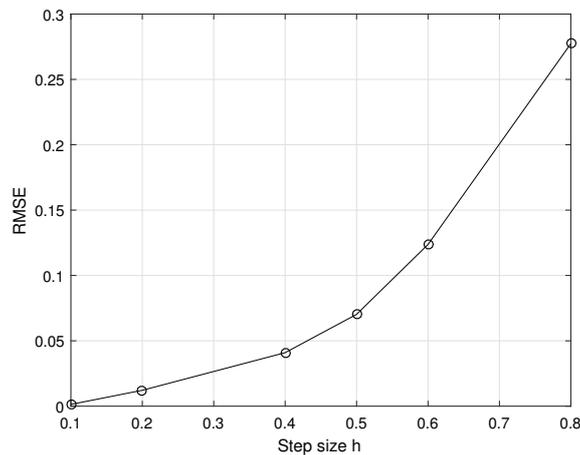


Figure 7: Absolute error ϵ_h of the proposed method in Example 2 for various h .

180 5. Conclusions

In this paper multidimensional DAR problems are solved by a proposed ETD method paying a special attention to the numerical analysis of the fully discretized scheme instead of the stability of the solution of the system of ODEs freezing spatial step sizes.

185 In fact, using logarithmic norm of matrices and properties of matrix exponential, sufficient condition on the step sizes are given, so that the numerical solution of the difference scheme remains norm bounded as the stepsizes tend to zero and the size of the involved matrices grows infinitely. Moreover, these conditions are sufficient for the positivity of the solution, that is important dealing
190 with real physical objects, as concentrations, populations, prices, etc.

Acknowledgements

This work has been partially supported by the Ministerio de Economía y Competitividad Spanish grant MTM2017-89664-P.

λ	P_h
0	3.6583
1	3.7869
10	3.9288
100	3.9730
1000	3.9732
10000	3.9733
Tree method (P)	3.9751

Table 4: Option price for the parameters (47).

Nodes	Proposed method	HOC
12×12	3.18982	2.86247
24×24	3.35338	3.27894
48×48	3.41344	3.35094

Table 5: American basket call option price comparison for Example 4.

References

- 195 [1] W. Hundsdorfer, J. Verwer, Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations, Springer Berlin Heidelberg, 2003.
- [2] F. Rossi, S. Ristori, M. Rustici, N. Marchettini, E. Tiezzi, Dynamics of pattern formation in biomimetic systems, Journal of Theoretical Biology 255 (4) (2008) 404 – 412.
- 200 [3] F. Yi, J. Wei, J. Shi, Bifurcation and spatiotemporal patterns in a homogeneous diffusive predatorprey system, Journal of Differential Equations 246 (5) (2009) 1944 – 1977.
- [4] J. Hull, Options, Futures and Other Derivatives, Pearson/Prentice Hall, 2009.

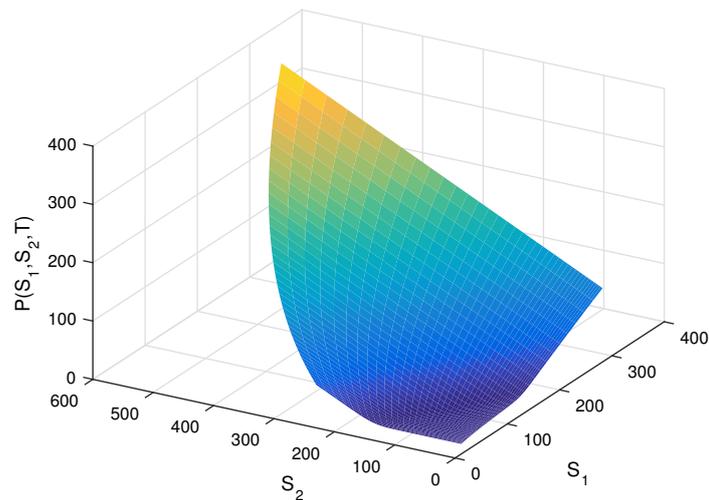


Figure 8: Basket call option price with parameters (50) at $\tau = T$.

- 205 [5] D. A. Garzón-Alvarado, C. Galeano, J. Mantilla, Computational examples of reaction–convection–diffusion equations solution under the influence of fluid flow: First example, *Applied Mathematical Modelling* 36 (10) (2012) 5029 – 5045.
- [6] B. Gustafsson, H. O. Kreiss, J. Oliger, *Time-Dependent Problems and*
 210 *Difference Methods*, John Wiley & Sons, Inc., 1995.
- [7] M. G. Crandall, H. Ishii, P.-L. Lions, User’s guide to viscosity solutions of second order partial differential equations, *Bulletin of the American Mathematical Society* 27 (1992) 1–67.
- [8] E. Cokca, A computer program for the analysis of 1-d contaminant mi-
 215 *gration through a soil layer*, *Environmental Modelling & Software* 18 (2) (2003) 147 – 153.
- [9] M. Calvo, J. de Frutos, J. Novo, Linearly implicit Runge–Kutta methods

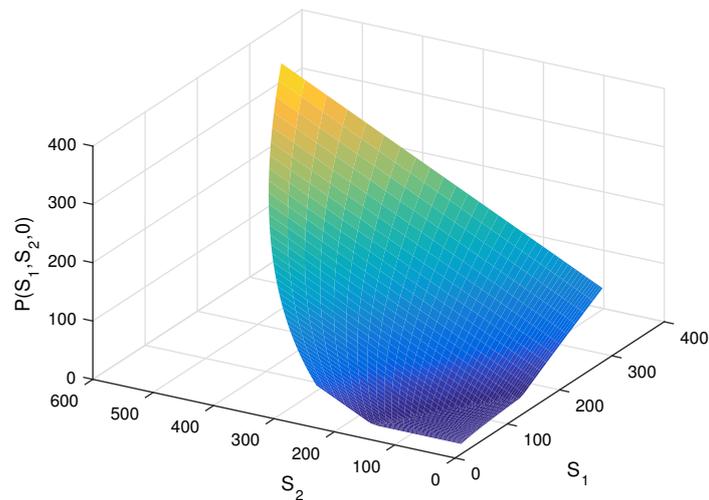


Figure 9: Basket call option price with parameters (50) at $\tau = 0$.

for advection–reaction–diffusion equations, *Applied Numerical Mathematics* 37 (4) (2001) 535 – 549.

- 220 [10] J. Macías-Díaz, A. Puri, An explicit positivity-preserving finite-difference scheme for the classical Fisher–Kolmogorov–Petrovsky–Piscounov equation, *Applied Mathematics and Computation* 218 (9) (2012) 5829 – 5837.
- [11] A. Kaya, Finite difference approximations of multidimensional unsteady convectiondiffusionreaction equations, *Journal of Computational Physics* 285 (2015) 331–349.
- 225 [12] S. Cox, P. Matthews, Exponential time differencing for stiff systems, *Journal of Computational Physics* 176 (2) (2002) 430 – 455.
- [13] F. de la Hoz, F. Vellido, Numerical simulations of time-dependent partial differential equations, *Journal of Computational and Applied Mathematics* 295 (2016) 175 – 184.
- 230

- [14] A.-K. Kassam, L. N. Trefethen, Fourth-order time-stepping for stiff pdes, SIAM Journal on Scientific Computing 26 (4) (2005) 1214–1233.
- [15] N. Rambeerich, D. Tangman, M. Lollchund, M. Bhuruth, High-order computational methods for option valuation under multifactor models, European Journal of Operational Research 224 (1) (2013) 219 – 226.
- [16] K. E. Atkinson, An Introduction to Numerical Analysis, John Wiley & Sons, Inc., 1989.
- [17] T. Kaczorek, Positive 1D and 2D Systems, Springer London, 2002.
- [18] G. Dahlquist, Stability and error bounds in the numerical integration of ordinary differential equations, Almqvist & Wiksells, Uppsala, 1958; Transactions of the Royal Institute of Technology, Stockholm.
- [19] C. A. Desoer, M. Vidyasagar, Feedback Systems: Input–Output Properties, Academic Press, 1975.
- [20] R. A. Fisher, The wave of advance of advantageous genes, Annals of Eugenics 7 (4) (1937) 355–369.
- [21] A. Kolmogorov, N. Petrovsky, S. Piscounov, tude de lquations de la diffusion avec croissance de la quantite de matiere et son application a un probleme biologique, Bull. Univ. Moskou 1 (1937) 1–25.
- [22] P. K. Brazhnik, J. J. Tyson, On traveling wave solutions of Fisher’s equation in two spatial dimensions, SIAM Journal on Applied Mathematics 60 (2) (1999) 371–391.
- [23] W. Qin, D. Ding, X. Ding, Two boundedness and monotonicity preserving methods for a generalized Fisher-KPP equation, Applied Mathematics and Computation 252 (2015) 552 – 567.
- [24] D. Tavella, C. Randall, Pricing Financial Instruments: The Finite Difference Method, John Wiley and Sons, New York, 2007.

- [25] P. A. Forsyth, K. R. Vetzal, Quadratic convergence for valuing american options using a penalty method, *SIAM Journal of Scientific Computing* 23 (2002) 2095–2122.
- 260 [26] B. F. Nielsen, O. Skavhaug, A. Tveito, Penalty methods for the numerical solution of American multi-asset option problems, *Journal of Computational and Applied Mathematics* 222 (1) (2008) 3 – 16, special Issue: Numerical {PDE} Methods in Finance.
- [27] K. S. T. Gad, J. L. Pedersen, Rationality parameter for exercising American put, *Risks* 3 (2) (2015) 103.
- 265 [28] R. Company, V. Egorova, L. Jódar, C. Vázquez, Finite difference methods for pricing american put option with rationality parameter: Numerical analysis and computing, *Journal of Computational and Applied Mathematics* 304 (2016) 1–17.
- 270 [29] R. Company, V. Egorova, L. Jódar, F. Soleymani, A mixed derivative terms removing method in multi-asset option pricing problems, *Applied Mathematics Letters* 60 (2016) 108 – 114.
- [30] S. Borovkova, F. Permana, J. van der Weide, American basket and spread option pricing by a simple binomial tree, *The Journal of Derivatives Summer* (2012) 29–38.
- 275